Oxygen Plasma Modeling in Dielectric Barrier Discharge by Using Comsol Multiphysics

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Modeling of Dielectric Barrier Discharge allow for the study of basic plasma processes, and also enable analysis and optimization of current technologies using plasmas, as well as predicting the performance of as-yet-unbuilt systems for new applications. Modeling of Dielectric Barrier Discharge (DBD) allow for the study of basic plasma processes, and also enable analysis and optimization of current technologies using plasmas, as well as predicting the performance of as-yet-unbuilt systems for new applications. These discharges are sometimes called silent discharges; usually operate at frequencies between 0.05 and 500 kHz. It is known that DBD generates non-thermal equilibrium plasma even under atmospheric pressure, which is suitable for ozone production [1]. Copious quantities of reactive oxygen species are often generated in atmospheric pressure plasmas. The reactive species and amounts generated depend on plasma parameters, such as the rotational, vibrational, excitation temperature and electron density [2].

This work represents a contribution of modeling of Dielectric Barrier Discharge in oxygen by using Comsol Multiphysics software, the powered electrode is driven by sinusoidal high voltage under 50 kHz of frequency, and the chemical model contains 75 reactions with a various species, where the electron collision with the heavy species included in this work are taken from the references [3.4]. The simulation results show an ozone molecules density and oxygen density and the others species.

Key words: Dielectric Barrier Discharge, oxygen plasma, fluid modeling, Comsol Multiphysics.

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Abstract

A one Dimension symmetric DBD model was developed, for the reason of ozone generation, using a sinusoidal high voltage. Simulation result show an ozone molecules density and oxygen density and the others species. The model contain 75 reactions with a various species consisting to evaluate the model and getting an optimum result. The numerical model used in this work was described in abridgement.

Introduction

Ozone is a powerful disinfecting and oxidizing agent, and for this reason, it is used in a wide range of applications such as treatment of municipal and wastewater, food processing, fire restoration, restoration of buildings and other objects after floods, etc. When ozone is exposed to organic compounds or bacteria, the extra atom of oxygen destroys the contaminant by oxidation [1].

Ozone generation with Dielectric Barrier Discharge DBD device is an interesting search subject for the advantages of DBD's including the low gas flow needed, the homogeneous discharges ignited over comparably big area together with different geometries of electrode leading to good adaptability [2].

Ozone is usually generated between two metallic electrodes, of which one electrode is covered with dielectric, using an ac or dc high voltage. DBD discharges, which are sometimes called silent discharges, usually operate at frequencies between 0.05 and 500 kHz. It is known that DBD generates a non-thermal equilibrium plasma even under atmospheric pressure, which is suitable for ozone production. [3].

Modeling of DBD allow for the study of basic plasma processes, but also enable analysis and optimization of current technologies using plasmas, as well as predicting the performance of as-yet-unbuilt systems for new applications.[5]

Copious quantities of reactive oxygen species are often generated in atmospheric pressure plasmas. The reactive species and amounts generated depend on plasma parameters, such as the rotational, vibrational, excitation temperature and electron density.[6]

This proposed model include plasma chemistry, surface reactions, density of electrons and heavy species (ions, atom…), electric failed, for better understanding DBDs at atmospheric pressure in O_2.

DESCRIPTION OF THE MODEL

A. *Electron Transport*

The continuity equation for the electron density is given by:

$$\frac{\partial n_e}{\partial t} + \nabla.\Gamma_e = R_e \qquad (1)$$

$$\Gamma_e = -\mu_e E n_e - \nabla(D_e n_e) \qquad (2)$$

With: n_e: Electron density $(1/m^3)$, R_e: Electron rate expression $(1/m^3.s)$, μ_e: Electron mobility $(m^2/V.s)$, E : Electric field (V/s), D_e: Electron diffusivity (m^2/s) and e : refers to electron.

Electron energy is given by:

$$\frac{\partial n_\varepsilon}{\partial t} + \nabla.\Gamma_\varepsilon + E.\Gamma_e = R_\varepsilon \qquad (3)$$

$$\Gamma_\varepsilon = -\mu_\varepsilon E n_\varepsilon - \nabla(D_\varepsilon n_\varepsilon) \qquad (4)$$

With:
n_ε: Electron energy density (V/m^3), R_ε: Energy loss/gain due to inelastic collisions $(V/(m^3.s))$, μ_ε: Electron energy mobility $(m^2/V.s)$, D_ε: Electron energy diffusivity (m^2/s) and ε : refers to energy.

Electron energy, ε (V) computed by:

$$\varepsilon = \frac{n_\varepsilon}{n_e} \qquad (5)$$

The source coefficients in the above equations are determined by the stoichiometry of the system and are written using either rate coefficients or Townsend coefficients [4].

Suppose that there are M reactions which contribute to the growth or decay of electron density and P inelastic electron-neutral collisions [4].

The electron energy loss is obtained by summing the collisional energy loss over all reactions:

$$R_e = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j \qquad (6)$$

With: P: inelastic electron-neutral collisions; x_j: Mole fraction of the target species for reaction j; k_j: Rate coefficient for reaction j (m^3/s); N_n: Total neutral number density ($1/m^3$) and $\Delta\varepsilon_j$: Energy loss from reaction j (V);

The Townsend coefficients k_j depend exponentially on the mean electron energy, ε . When a Maxwellian EEDF is assumed, the Townsend coefficients can be fitted with a function of the form:

$$k_j = A\varepsilon^{\beta} e^{-E/\varepsilon} \qquad (7)$$

A. *Electrostatics Equations*

- Electrostatic field :

$$-\nabla.\varepsilon_0.\varepsilon_r \nabla V = \rho \qquad (8)$$

- The space charge density :

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right) \qquad (9)$$

- The constitutive relation :

$$D = \varepsilon_0 \varepsilon_r E \qquad (10)$$

This relation (9) describe the macroscopic properties of the dielectric coating medium (relating the electric displacement D with the electric field E) and the applicable material properties.

- Surface charge accumulation is added to boundaries by way of the following boundary condition:

$$-n.(D_1 - D_2) = \rho_s \qquad (11)$$

where ρ_s is the solution of the following distributed ODE on the boundary:

$$\frac{d\rho_s}{dt} = n.J_i + n.J_e \qquad (12)$$

Where $n.J_i$ and $n.J_e$ are the normal component of the total ion current density and the total electron current density respectively on the wall.

PLASMA CHEMISTRY

In this part of our work is an aggregation of possible chemical reactions in oxygen O_2 as a gas filled in discharge gap.

Electron impact reactions : The cross section set for electron collisions in O_2 used in this calculation is shown in Tab.1 [7.8].

Reactions and rate coefficient in Tab.2, and the wall reactions in the table 3.

TABLE I. Phelps databases

Reaction	*Formula*	*Reaction*	*Formula*
1	e+ O_2=>e+ O_2	*16*	e+O2b1s=>e+O2b1s
2	e+ O_2=>O+O^-	*17*	e+O2b1s=>e+O+O
3	e+ O_2=>e+O2a1d	*18*	e+O2b1s=>2e+ O_2^+
4	e+O2a1d=>e+ O_2	*19*	e+O245=>e+O+O
5	e+ O_2=>e+O2b1s	*20*	e+O245=>2e+ O_2^+
6	e+O2b1s=>e+ O_2	*21*	e+O=>e+O
7	e+ O_2=>e+O245	*22*	e+O=>e+O1d
8	e+O245=>e+ O_2	*23*	e+O1d=>e+O
9	e+ O_2=>e+O+O	*24*	e+O=>e+O1s
10	e+ O_2=>e+O+O1d	*25*	e+O1s=>e+O
11	e+ O_2=>e+O+O1s	*26*	e+O=>2e+O^+
12	e+ O_2=>2e+ O_2^+	*27*	e+O1d=>e+O1s
13	e+O2a1d=>e+O2a1d	*28*	e+O1d=>2e+O^+
14	e+O2a1d=>e+O+O	*29*	e+O1s=>2e+O^+
15	e+O2a1d=>2e+ O_2^+	*30*	e+ O_3=>e+O_3
16	e+O2b1s=>e+O2b1s	*31*	e+ O_3=>O^-+ O_2
17	e+O2b1s=>e+O+O	*32*	e+ O_3=>2e+O_3^+

TABLE II. Most important reactions

Formula	Rate constant k^f	Formula	Rate constant k^f
e+O_2^+ → O+O	5.2e-9/T_e	O2a1d+O → O_2+O	2e-22
e+O_2^+ → O+O1d	1.95e-13*(Te/300)^-0.7	O2a1d+O_3 → O_2+ O_2+O	52e-18*exp(-2839/Te)
e+O^+ → O	1.3978e-16*Te^-0.66	O2b1s+ O_2 → O_2+ O_2	2.317e-28*Te^0.5
e+O_2+O_2 → O_2^-+O_2	3.6e-40*Te^-0.5	O2b1s+O → O_2+O	4.634e-22*Te^0.5
O^++O_2 → O+O_2+	1.9e-18*Te^-0.4	O245+ O_2 → O_2+ O_2	2e-19
O^-+O2a1d → O_2^-+O_2	7.3e-16*exp(-890/Te)	O1d+O_3 → O_2+ O_2	1.2e-16
O^-+O2a1d → O_3+e	7e-16	O1d+O_3 → O_2+O+O	1.2e-16
O_2^-+O2a1d → O_2+O_2+e	6.7e-17	O1d+ O_2 → O_2+O	3.2e-17*exp(67/Te)
O_2^-+ O_2^+ → O_2+O_2	4.2e-7	O1d+O → O+O	8e-18
O_2^-+O+ → O_2+O	2e-7*(Te/300)^-0.5	O1s+O_3 → O_2+ O_2	4.63e-16
O_2^-+ O_3+ → O_2+ O_3	751e-16*(Te/300)^-0.5	O1s+ O_2 → O_2+O	4.8e-18*exp(67/Te)
O^-+ O_3+ → O+ O_3	751e-16*(Te/300)^-0.5	O1s+O → O+O	3.33e-17*exp(-300/Te)
O^-+ O_2^+ → O+ O_2	1.48e-16*(Te/300)^-0.5	O+O_3 → O_2+ O_2	8e-18*exp(-2060/Te)
O^-+O+ → O+O	2.35e-7*(Te/300)^-0.5	O+O+ O_2 → O_2+ O_2	9.268e-42*Te^-0.63
O^-+O → O_2+e	1.9e-16	O+O+O → O_2+O	3.33e-41*Te^-0.63
O+ O_2+ O_2 → O_3+O_2	6e-46*(Te/300)^-2.4	O+e → O^-	1.5e-15
O2a1d+ O_2 → O_2+ O_2	3e-24*exp(-200/Te)	O^-+O2a1d → O_2^-+O	7.30e-10*exp(890/Te)

TABLE III. Surface reactions

Reaction	*Formula*
1	O_2^+→O_2
2	O^+→O
3	O_3^+→O_3
4	O2a1d→ O_2
5	O2b1s→ O_2
6	O245→ O_2
7	O1d→O
8	O1s→O
9	O_2^-→ O_2
10	O-→O

Results

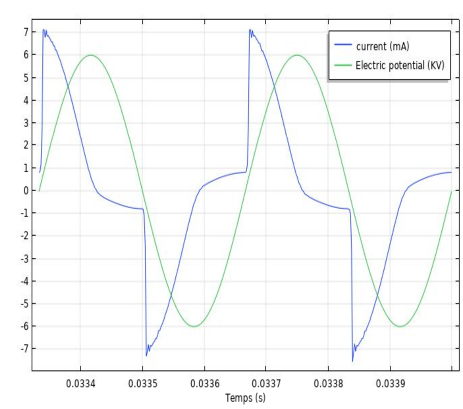

Fig.1. applied Voltage and output current

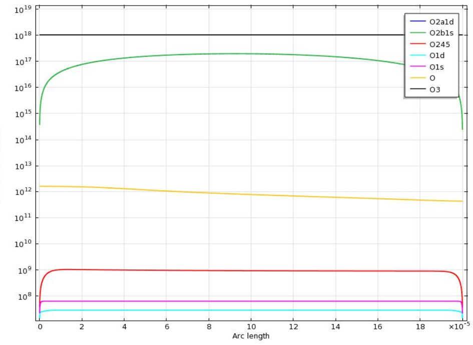

Fig.2. Neutral species densities

Result Discussion

When the voltage applied (Fig.2) to the high voltage wire, an electric field forms in the gap. Free electrons in the gap will be accelerated and may acquire enough energy to cause ionization. The newly created electrons rush towards the grounded dielectric circle. An equal number of ions are also created since the electrons and ions must be created in equal pairs. The ions rush towards the dielectric circle where the voltage is being applied with negative polarity.

From Figure 2, it can be understood that there is a great rise in number densities of electron and Oxygen ions the ions and free electrons concentration is near the dielectric coatings connected to high voltage that means until this time avalanches occur in this area. However as the applied voltage increases, a stronger electric field forms in the gap between electrodes and any free electron in the gap will be accelerated and since the electric field is strong enough they acquire enough energy to cause significant ionization activities that means avalanches occurs in across the gap uniformly

Conclusion

For a large-scale of using ozone in servile industrial and medical applications, ozone is mainly prepared by non-thermal plasma technologies based on electrical discharges.

This paper develops model to study ozone generation by DBD. It simulated with a relatively complete physico-chemical model that includes elementary plasma processes and chemical reactions between discharge species.

The results of the simulation have shown the time evolution of species concentration in gap.

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